

Michela Taufer

University of Delaware
Department of Computer and Information Science
103 Smith Hall
Newark, DE 19716

Phone: (302) 831 0071
Fax: (302) 747 5030
E-Mail: mtaufer@acm.org

Personal Homepage: <http://cis.udel.edu/~taufer>
Research Group Homepage – Global Computing Lab: <http://gcl.cis.udel.edu>

Education

- Dec 2002 PhD in Computer Science, Swiss Federal Institute of Technology Zurich (ETH), Switzerland.
Thesis: ***Inverting Middleware: Performance Analysis of Layered Application Codes in High Performance Distributed Computing.***
Thesis supervisors: Thomas M. Stricker (Chair), Daniel A. Reed
- Dec 1996 MS in Computer Engineering, University of Padua, Italy.
Thesis: ***Development of the Parallelization of the Software Package OPAL for the Simulation of Dynamic Molecules on Supercomputers.***
Thesis supervisors: Gianfranco Bilardi (Chair), Walter Gander, Geppino Pucci

Research Interests

Grid and volunteer computing systems; multi-scale dynamic-data-driven adaptive modeling and simulation in biomedical sciences; adaptive and dynamically reconfigurable systems for bioinformatics applications; tools for data access and management, data analysis, and data visualization in grid and volunteer computing environments; parallelization, performance analysis, and optimization of scientific applications.

Professional Experience

- Sep 2007 - present Assistant professor and leader of the Global Computing Laboratory at the Department of Computer and Information Sciences, University of Delaware, Newark, USA.
- Jan 2005 – Aug 2007 Assistant professor and leader of the Global Computing Laboratory at the Department of Computer Science, University of Texas, El Paso, USA.
- Jan 2003 – Dec 2004 Postdoctoral researcher at the Center for Theoretical Biological Physics (CTBP), University of California, San Diego. Affiliated to the Department of Molecular Biology at The Scripps Research Institute (TSRI), the San Diego Supercomputer Center (SDSC), and the Department of Computer Science and Engineering at the University of California at San Diego.
- Dec 1996 – Dec 2002 Research student assistant at the Computer Systems Institute, Swiss Federal Institute of Technology Zurich (ETH), Switzerland.
- Feb 1996 – Dec 1996 Visitor scholar at the Swiss Center for Scientific Computing (SCSC/CSCS), Zurich, Switzerland.

Publications and Presentations

Journal Articles:

- [1] M. Tauffer, R.S. Armen, J. Chen, P.J. Teller, and C.L. Brooks III: **Computational Multi-Scale Modeling in Protein-Ligand Docking**. Submitted to the *IEEE Engineering in Medicine and Biology Magazine*, 2008.
- [2] M. Tauffer, M.-Y. Leung, A. Licon, D. Mireles, T. Solorio, D. Gomez-Leon, R. Araiza, K.K. Johnson: **RNAVLab: A unified environment for computational RNA structure analysis based on grid computing technology**. Submitted to the *Journal of Parallel Computing*, 2007.
- [3] K. Bhatia, M. Tauffer, B. Stearn, R. Zamudio, and D. Catarino: **Integrate GridFTP into Firefox - Build grid protocols into Mozilla-based tools**. *IBM developerWorks*, October 2006.
- [4] M. Tauffer, C. An, A. Kerstens, and C.L. Brooks III: **Predictor@Home: A Protein Structure Prediction Supercomputer Based on Global Computing**. *IEEE Transactions on Parallel and Distributed Systems*, Volume: 17, Issue: 8, Pages: 786- 796, August 2006.
- [5] M. Tauffer, M. Crowley, D. Price, A.A. Chien, and C.L. Brooks III: **Study of an Accurate and Fast Protein-Ligand Docking Algorithm based on Molecular Dynamics**. *Concurrency and Computation: Practice and Experience*. Volume 17, Issue 14, Pages: 1627-1641, December 2005.
- [6] P. Cicotti, M. Tauffer, and A.A. Chien: **DGMonitor: a Performance Monitoring Tool for Sandbox-based Desktop Grid Platforms**. *Journal of Supercomputing*, Springer Science+Business Media B.V., Formerly Kluwer Academic Publishers B.V. Issue 34, Number 2, Pages: 113 – 133, November 2005.
- [7] K. Baldridge, J.P. Greenberg, W. Sudholt, K. Bhatia, S. Mock, C. Amoreira, Y. Potier, and M. Tauffer: **The Computational Chemistry Prototyping Environment**. *IEEE Special Issue on Grid Computing*, Volume: 93, Issue: 3, Pages: 510 – 521, March 2005.

Research Papers in Refereed Conferences, Symposiums, and Workshops (peer-reviewed):

- [1] T. Estrada, O. Fuentes, and M. Tauffer: **A Distributed Evolutionary Method to Design Scheduling Policies for Volunteer Computing**. To appear in the *Proceedings of ACM Computing Frontiers 2008*, May 2008, Ischia, Italy. (30/110, 27%)
- [2] M. Tauffer, T. Solorio, A. Licon, D. Mireles, and M.-Y. Leung: **On the Effectiveness of Rebuilding RNA Secondary Structures from Sequence Chunks**. To appear in *Proceedings of the Seventh IEEE International Workshop on High Performance Computational Biology (HiCOMB'08)*, April 2008, Miami, Florida, USA.
- [3] G. Lopez, M. Tauffer, and P.J. Teller: **Evaluation of IEEE 754 Floating-Point Arithmetic Compliance Across a Wide Range of Heterogeneous Computers**. In *Proceedings of the 2007 Richard Tapia Celebration of Diversity in Computing Conference*, October 2007, Orlando, Florida, USA.
- [4] R. Araiza, M. Tauffer, and M.-Y. Leung: **Towards Optimal Scheduling for Global Computing Under Probabilistic, Interval, and Fuzzy Uncertainty, with Potential Applications to Bioinformatics**. In *Proceedings of the 26th International Conference of the North American Fuzzy Information Processing Society (NAFIPS'2007)*, June 2007, San Diego, California.
- [5] M. Tauffer, A. Kerstens, T. Estrada, D.A. Flores, and P.J. Teller: **SimBA: a Discrete Event Simulator for Performance Prediction of Volunteer Computing Projects**. In *Proceedings of the International Workshop on Principles of Advanced and Distributed Simulation 2007 (PADS'07)*, June 2007, San Diego, California, USA. (65%)
- [6] M. Tauffer, M.-Y. Leung, K.L. Johnson, and A. Licon: **RNAVLab: A Unified Environment for Computational RNA Structure Analysis based on Grid Computing Technology**. In *Proceedings of the Sixth IEEE International Workshop on High Performance Computational Biology (HiCOMB'07)*, March 2007, Long Beach, California, USA.
- [7] M. Tauffer, A. Kerstens, T. Estrada, D.A. Flores, R. Zamudio, P.J. Teller, R. Armen, and C.L. Brooks III: **Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling**

- and Scheduling.** In *Proceedings of the First Workshop on Large-Scale, Volatile Desktop Grids (PCGrid'07)*, March 2007, Long Beach, California, USA.
- [8] R. Zamudio, D. Catarino, M. Taufer, K. Bhatia, and B. Stearn: **Topaz: Extending Firefox to Accommodate the GridFTP Protocol.** In *Proceedings of the Fourth High-Performance Grid Computing Workshop (HPGC'07)*, March 2007, Long Beach, California, USA
- [9] T. Estrada, D. Flores, M. Taufer, P. Teller, A. Kerstens, and D.P. Anderson: **The Effectiveness of Threshold-based Scheduling Policies in BOINC Projects.** In *Proceedings of the Second IEEE International Conference on e-Science and Grid Technologies (eScience'06)*. December 2006, Amsterdam, The Netherlands.
- [10] T. Estrada, A. Licon, and M. Taufer: **CompPknots: a Framework for Parallel Prediction and Comparison of RNA Secondary Structures with Pseudoknots.** In *Proceedings of the First Workshop on High Performance Computing in Genomic, Proteomic and Transcriptomic (HPC GPT'06)*, in conjunction with ISPA'06, December 2006, Sorrento, Italy.
- [11] K. Bhatia, B. Stearn, M. Taufer, R. Zamudio, and D. Catarino: **Extending Grid Protocols onto the Desktop using the Mozilla Framework.** In *Proceedings of the Second IEEE/ACM International Workshop on Grid Computing Environments (GCE'06)*, in conjunction with SC'06, November 2006, Tampa, Florida, USA.
- [12] G. Aguilera, P.J. Teller, M. Taufer, and F. Wolf: **A Systematic Multi-step Methodology for Performance Analysis of Communication Traces of Distributed Applications based on Hierarchical Clustering.** In *Proceedings of the Fifth International Workshop on Performance Modeling, Evaluation, and Optimization of Parallel and Distributed Systems (PMEO-PDS'06)*, in conjunction with IPDPS'06, April 2006, Rhodes Island, Greece.
- [13] M. Taufer, P.J. Teller, D.P. Anderson, and C.L. Brooks III: **Metrics for Effective Resource Management in Global Computing Environments.** In *Proceedings of the First IEEE International Conference on e-Science and Grid Technologies (eScience'05)*. December 2005, Melbourne, Australia. (31.6%)
- [14] M. Taufer, C. An, A. Kerstens, and C.L. Brooks III: **Predictor@Home: A "Protein Structure Prediction Supercomputer" Based on Public-Resource Computing.** In *Proceedings of the Fourth IEEE International Workshop on High Performance Computational Biology (HiCOMB'05)*, in conjunction with IPDPS'05, April 2005, Denver, Colorado, USA.
- [15] M. Taufer, D.P. Anderson, P. Cicotti, and C.L. Brooks III: **Homogeneous Redundancy: a Technique to Ensure Integrity of Molecular Simulation Results Using Public Computing.** In *Proceedings of the Fourteenth Heterogeneous Computing Workshop (HCW'05)*, in conjunction with IPDPS'05, April 2005, Denver, Colorado, USA. (47%)
- [16] M. Taufer, M. Crowley, D. Price, A.A. Chien, and C.L. Brooks III: **Study of an Accurate and Fast Protein-Ligand Docking Algorithm based on Molecular Dynamics.** In *Proceedings of the Third IEEE International Workshop on High Performance Computational Biology (HiCOMB'04)*, in conjunction with IPDPS'04, April 2004, Santa Fe, New Mexico, USA.
- [17] D. Kondo, M. Taufer, C.L. Brooks III, H. Casanova, and A.A. Chien: **Characterizing and Evaluating Desktop Grids: An Empirical Study.** In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS'04)*, April 2004, Santa Fe, New Mexico, USA. (31.7%)
- [18] P. Cicotti, M. Taufer, and A.A. Chien: **DGMonitor: a Performance Monitoring Tool for Sandbox-based Desktop Grid Platforms.** In *Proceedings of the Third International Workshop on Performance Modeling, Evaluation, and Optimization of Parallel and Distributed Systems (PMEO-PDS'04)*, in conjunction with IPDPS'04, April 2004, Santa Fe, New Mexico, USA.
- [19] M. Taufer, and T. Stricker: **A Performance Monitor based on Virtual Global Time for Clusters of PCs.** In *Proceedings of the IEEE International Conference on Cluster Computing 2003 (Cluster'03)*, December 2003, Hong Kong, China. (48/164, 29.3%)
- [20] B. Uk, M. Taufer, T. Stricker, G. Settanni, A. Cavalli, and A. Caflisch: **Combining Task- and Data Parallelism to Speed up Protein Folding on a Desktop Grid Platform - Is efficient protein folding**

- possible with CHARMM on the United Devices MetaProcessor?** In *Proceedings the IEEE International Symposium on Cluster Computing and the Grid (CCGRID'03)*, May 2003, Tokyo, Japan. (39/114, 34.2%)
- [21] B. Uk, M. Taufer, T. Stricker, G. Settanni, and A. Cavalli: **Implementation and Characterization of Protein Folding on a Desktop Computational Grid – Is CHARMM a suitable candidate for the United Devices MetaProcessor?** In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS'03)*, April 2003, Nice, France. (119/407, 29.2%)
- [22] M. Taufer, T. Stricker, and R. Weber: **Scalability and Resource Usage of an OLAP Benchmark on Clusters of PCs.** In *Proceedings of the Fourteenth ACM Symposium on Parallel Algorithms and Architectures (SPAA'02)*, August 2002, Winnipeg, Manitoba, Canada.
- [23] M. Taufer, T. Stricker, G. Roos, P. Guentert: **On the Migration of the Scientific Code DYANA from SMPs to Clusters of PCs and on to the Grid.** In *Proceedings of the IEEE International Symposium on Cluster Computing and the Grid (CCGRID'02)*, May 2002, Berlin, Germany. (25.0%)
- [24] M. Taufer, E. Perathoner, A. Cavalli, A. Caflich, and T. Stricker: **Performance Characterization of a Molecular Dynamics Code on PC Clusters - Is there any easy parallelism in CHARMM?** In *Proceedings of the IEEE/ACM International Parallel and Distributed Processing Symposium (IPDPS'02)*, April 2002, Fort Lauderdale, Florida, USA. (98/258, 38%)
- [25] M. Taufer, and T. Stricker: **Accurate Performance Evaluation, Modeling and Prediction of a Message Passing Simulation Code based on Middleware.** In *Proceedings of the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC'98)*, November 1998, Orlando, Florida, USA.
- [26] P. Arbenz, M. Billeter, P. Guentert, P. Luginbuehl, M. Taufer, and U. von Matt: **Molecular Dynamics Simulations on Cray Clusters using the Sciddle-PVM Environment.** Lecture Notes in Computer Science 1156 A. Bode, J. Dongarra, T. Ludwig, V. Sunderam (Eds.) *Presented at the Parallel Virtual Machine - EuroPVM 96, Third European PVM Conference*, October 1996, Munich, Germany.

Book Chapter:

- [1] M. Taufer and C.L. Brooks III: **Predictor@Home: A Protein Structure Prediction Supercomputer Based on Volunteer Computing.** In *Distributed & Grid Computing - Science Made Transparent for Everyone. Principles, Applications and Supporting Communities.* Tectum Verlag. (In Press, 2007).

Educational Papers:

- [1] M. Taufer, P.J. Teller, A. Kerstens, R. Romero: **Collaborative Research Tools for Students, Staff, and Faculty.** In *Proceedings of the International SUN Conference on Teaching and Learning*, March 2006, El Paso, Texas, USA.

Abstracts:

- [1] An, M. Taufer, and C.L. Brooks III: **Predictor@Home: A Multiscale, Distributed Approach for Protein Structure Prediction.** In *Proceedings of the 6th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP6)*, December 2004, Gaeta, Italy.

Posters:

- [1] T. Estrada, M. Taufer, and K. Reed: **Performance Analysis of Volunteer Computing Traces.** In *Proceedings of the ACM/IEEE International Conference for High Performance Computing, Network, Storage, and Analysis conference (SC'07)*, November 2007, Reno, Nevada, USA. (24.5%)
- [2] D. Flores, T. Estrada, M. Taufer, P. Teller, and A. Kerstens: **SimBA: a Discrete Event Simulator for Performance Prediction of Volunteer Computing Projects.** Poster in *Proceedings of the ACM/IEEE International Conference for High Performance Computing and Communications conference (SC'06)*, November 2006, Tampa, Florida, USA. (25%)
- [3] C. An, M. Taufer, and C.L. Brooks III: **Predictor@home: A Multiscale, Distributed Approach for**

Protein Structure Prediction. Poster presented at *the 229th ACM National Meeting*, March 2005, San Diego, California, USA

- [4] C. An, M. Taufer, and C.L. Brooks III: **Predictor@home: A Multiscale, Distributed Approach for Protein Structure Prediction.** Poster presented at *the 6th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP6)*, December 2004, Gaeta, Italy.

Technical Reports:

- [1] T. Estrada, A. Licon, and M. Taufer: **CompPknots: a Framework for Parallel Prediction and Comparison of RNA Secondary Structures with Pseudoknots.** Technical Report UTEP-CS-06-42, University of Texas, El Paso, September 2006.
- [2] T. Estrada, D. Flores, M. Taufer, P. Teller, A. Kerstens, and D. Anderson: **The Effectiveness of Threshold-based Scheduling Policies.** Technical Report UTEP-CS-06-30, University of Texas, El Paso, August 2006.
- [3] R. Zamudio, D. Catarino, M. Taufer, B. Stearn, and K. Bhatia: **Topaz: a Firefox Protocol Extension for GridFTP based on Data Flow Diagrams.** Technical Report UTEP-CS-06-18, University of Texas, El Paso, April 2006.
- [4] D. Kondo, M. Taufer, J. Karanicolas, C.L. Brooks III, H. Casanova, and A.A. Chien: **Characterizing and Evaluating Desktop Grids: An Empirical Study.** Technical Report CS2003-069, University of California, San Diego, November 2003.
- [5] P. Cicotti, M. Taufer, and A.A. Chien: **DGMonitor: a Performance Monitoring Tool for Sandbox-based Desktop Grid Platforms.** Technical Report CS2003-070, University of California, San Diego, November 2003.
- [6] B. Uk, M. Taufer, T. Stricker, G. Settanni, A. Cavalli, and A. Caflich: **Combining Task- and Data Parallelism to Speed up Protein Folding on a Desktop Grid Platform - Is efficient protein folding possible with CHARMM on the United Devices MetaProcessor?** Technical Report 386, Department of Computer Science, Swiss Federal Institute of Technology Zurich (ETH), November 2002.
- [7] B. Uk, M. Taufer, T. Stricker, G. Settanni, and A. Cavalli: **Implementation and Characterization of Protein Folding on a Desktop Computational Grid – Is CHARMM a suitable candidate for the United Devices MetaProcessor?** Technical Report 385, Department of Computer Science, Swiss Federal Institute of Technology Zurich (ETH), October 2002.
- [8] M. Taufer, T. Stricker, and R. Weber: **Inverting Middleware Framework: Framework for Performance Analysis of Distributed OLAP Benchmarks on Clusters of PCs by Filtering and Abstracting Low Level Resource Usage.** Technical Report 367, Department of Computer Science, Swiss Federal Institute of Technology Zurich (ETH), March 2002.
- [9] P. Arbenz, T. Stricker, M. Taufer, and U. von Matt: **Performance Characterization and Modeling of the Molecular Simulation Code OPAL.** Technical Report 310, Department of Computer Science, Swiss Federal Institute of Technology Zurich (ETH), November 1998.

Theses:

- [1] M. Taufer: **Inverting Middleware: Performance Analysis of Layered Application Codes in High Performance Distributed Computing.** Dissertation ETH No. 14845, Institute for Computer Systems, Swiss Federal Institute of Technology Zurich (ETH), December 2002, Zurich, Switzerland. Published by Hartung Gorre Verlag Konstanz, Germany, ISBN 3-89649-821-5 ISSN 1611-0943.
- [2] M. Taufer: **Development of the Parallelization of the Software Package OPAL for the Simulation of Dynamic Molecules on Supercomputers.** Master Thesis, Department of Computer Science, University of Padova, December 1996, Padova, Italy.

Selected Invited Talks:

- Jan 2008* 20th Annual CSU Biotechnology Symposium Information, Special Session on Interface between Computer Science and Biotechnology, Oakland California.
Title: *Computational Multi-Scale Modeling in Protein-Ligand Docking.*
- Oct 2007* Delaware Bioinformatics Institute, Newark, Delaware.
Title: *RNAVLab: A unified environment for computational RNA structure analysis based on grid computing technology.*
- Apr 2007* High Performance Computing Across Texas (HiPCAT) Meeting, El Paso, Texas.
Title: *RNAVLab: A unified environment for computational RNA structure analysis based on grid computing technology.*
- Mar 2007* Mississippi State University, Starkville, Mississippi.
Title: *Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling.*
- Mar 2007* University of Delaware, Newark, Delaware.
Title: *Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling.*
- Mar 2007* University of Pittsburgh, Pittsburgh, Pennsylvania.
Title: *Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling.*
- Mar 2007* University of New Mexico, Albuquerque, New Mexico.
Title: *Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling.*
- Feb 2007* University of South Florida, Tampa, Florida.
Title: *Moving Volunteer Computing towards Knowledge-Constructed, Dynamically-Adaptive Modeling and Scheduling.*
- Dec 2006* San Antonio Cancer Institute Seminar Series - via AccessGrid
Title: High-Performance Computing: An increasingly powerful tool for Biomedical Science - what can it do for Cancer Research?
- Oct 2006* The 19th Rocky Mountain Regional Meeting of The American Chemical Society, Tucson, Arizona.
Title: *Predictor@Home: A "Protein Structure Prediction Supercomputer" Based on Volunteer Computing*
- Sep 2006* Computer Science Department, University of Houston, Houston, Texas.
Title: *Moving Volunteer Computing Towards Data-Driven, Knowledge-Constructed Capabilities*
- Apr 2006* High Performance Computing Center, Texas Tech University, Lubbock, Texas.
Title: *Bioinformatics Colloquium - Predictor@Home: A "Protein Structure Prediction Supercomputer" Based on Global Computing.*
- Feb 2006* Bioinformatics Colloquium, University of Texas at El Paso, El Paso, Texas.
Title: *Predictor@Home: A "Protein Structure Prediction Supercomputer" Based on Global Computing.*
- Dec 2005* National ICT Australia (NICTA), Sydney, Australia.
Title: *Metrics for Effective Resource Management in Global Computing Environments.*
- May 2004* Department of Computer Science, University of Lugano, Switzerland.
Title: *Desktop Grid Computing: a Virtual Laboratory for Studying Complex Phenomena in Nature.*
- Mar 2004* Department of Computer Science, University of Texas, El Paso, Texas.
Title: *Desktop Grid Computing: a Virtual Laboratory for Studying Complex Phenomena in Nature.*

- Apr 2003* Department of Biochemistry, University of Zurich, Switzerland.
Title: *The Desktop Grid – A Flexible Platform for Bioinformatics.*
- Apr 2003* Department of Computer Science, Swiss Federal Institute of Technology Zurich (ETH), Switzerland.
Title: *The Desktop Grid – A Flexible Platform for Bioinformatics.*
- Nov 2002* Department of Computer Science and Engineering (CSE), University of California, San Diego (UCSD), La Jolla, California.
Title: *Study of Viability and Effectiveness of CHARMM Applications on Distributed Systems.*
- Nov 2002* San Diego Supercomputer Center at UCSD, La Jolla, California.
Title: *Study of Viability and Effectiveness of CHARMM Applications on Distributed Systems.*
- Sep 2002* Department of Computer Science, Vrije Universiteit Amsterdam, The Netherlands.
Title: *Inverted Middleware: Performance Analysis of Layered Application Codes in Distributed Computing.*
- Aug 2002* Department of Computer Science, University College of London (UCL), United Kingdom.
Title: *The importance of Effective Performance Analysis – How to be successful in migrating existing applications to distributed systems.*

Invited Panel:

- Nov 2003* Invited speaker at the panel discussion: “The Great Academia/Industry Grid Debate”, Fourth International Workshop on Grid Computing (Grid 2003), Phoenix, Arizona.
Title: *What we DO need to make Desktop Grids a Success in Practice*

Funding and Awards

Research Grants:

- May 2007* SCORE- NIH - Funded awarded: \$581,329, co-PI
 Title: **Computational Prediction of RNA Viral Genome Structures**
 Description: Design and implementation of mathematical method and computation tools for RNA secondary structure prediction in viral genomics.
 Participants: Ming-Ying Lung (PI, UTEP) and Michela Taufer (co-PI)
 Duration: 09/01/2007- 08/31/2007
 Note: The grant was awarded to UTEP, a Minority Serving Institution (MSI). Because U. Delaware is not a MSI, my funds were not relocated to my new institutions, U Delaware.
- Apr 2007* Army HPC Research Center - Funded awarded: \$1,250,000, PI of subcontract
 Title: **P-L UniFrame: a unifying framework for adaptive protein-ligand docking on HPC systems**
 Description: The major goal of this project is to implement adaptive protein-ligand docking algorithms that run on high-performance systems efficiently.
 Participants: Michela Taufer (PI, UTEP) and Patricia J. Teller (co-PI, UTEP)
 Duration: 04/01/2007 – 04/30/2012
 Note: The University of Texas at El Paso withdrew the awarded project after my relocation to U. Delaware.
- May 2006* ARP grant #003661-0008-2006, Advanced Research Program (ARP) - Texas Higher Education Coordinating Board, Funds awarded \$99,982, PI
 Title: **RNA Secondary Structure Prediction Using a Grid of Heterogeneous Computers**
 Participants: Michela Taufer (PI, UTEP), Ming-Ying Leung (co-PI, UTEP)
 Duration: from May 15, 2006 to May 14, 2008
 Description of Project: Build an adaptive grid computing system that, at runtime, identifies and exploits computer resources across the University of Texas at El Paso (UTEP) campus to predict secondary structures of large numbers of RNA segments using a variety of prediction programs.
 Note: The grant was not relocated to U. Delaware.
- Sep 2005* NSF grant #0506429, SCI TESTBEDS, total funds \$1,220,036, awarded to UTEP \$655,626, PI
 Title: **Collaborative Research: DAPLDS - a Dynamically Adaptive Protein-Ligand Docking System based on Multi-Scale Modeling**
 Participants: Michela Taufer (PI), David P. Anderson (co-PI University of California-Berkeley), Charles L. Brook III (co-PI, The Scripps Research Institute), and Patricia J. Teller (subcontract, UTEP)
 Duration: from September 1, 2005 to August 31, 2008
 Description of Project: Exploration of the multi-scale nature of algorithmic adaptations in protein-ligand docking; and development of cyber infrastructures based on computational methods and models that efficiently accommodate these adaptations.

Educational Grants at UTEP:

- Oct 2006* NSF grant #0631168, DUE, total funds \$275,856 awarded to UTEP, PI
 Title: **SHIPPER: Spreading High-Performance computing Participation in undergraduate Education and Research**
 Participants: Michela Taufer (PI, UTEP), Patricia J. Teller (co-PI, UTEP)
 Duration: from October 1, 2006 to January 31, 2011
 Description of Project: Create and consolidate a community of UG and graduate students who will pursue advanced degrees in fields that combine expertise in high-performance computing and other scientific and engineering disciplines.
 Note: The grant was not relocated to U. Delaware.

Infrastructure Grants:

- Sep 2005* IBM Shared University Research (SUR) Award Program, over \$600,000 retail value, co-PI
Title: **Performance via Autonomicity, Analysis, Virtualization, and Micro-partitioning, and Research in Life Sciences and Bioinformatics**
Participants: P. Teller (PI), S. Aley (co-PI), L. Bain (co-PI), W. Baldwin (co-PI), F. Modave (co-PI), M.-Y. Leung (co-PI), P. Nava (co-PI), M. Taufer (co-PI), and D. Villa (co-PI)
Description of Project: Performance analysis and parallelization of the PKNOT code for RNA secondary structure predictions.
- Jul 2005* UTEP Seed Funds, \$23,400, co-PI
Title: **High-Performance Modular FEM/hp-FEM System (HERMES)**
Participants: Pavel Solin (PI), Michela Taufer (co-PI)

Academic Awards, Scholarships, and Fellowships:

- Jul 2006* NIH/PSC travel award to attend the workshop "MARC: Developing Bioinformatics Programs", Pittsburgh Supercomputing Center, July 17-28
- Apr 2006* College of Engineering Young Investigator Award (UTEP)
- Jan 2006* Software gift from Innobase Oy: perpetual InnoDB Hot Backup license for Linux
Award amount: \$1,300
- Dec 2005* Software gift from University of Harvard: CHARMM license for the DAPLDS project
Award amount: \$600
- Apr 2005* NSF travel award to attend the CRA Women Workshop for Women in Academic Career, Washington D.C., Virginia
- Dec 2004* Travel award to attend the 6th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP6), Gaeta, Italy
- Jan 2003* La Jolla Interfaces in Science (LJIS) Interdisciplinary Fellowship
From January 1, 2003 to December 14, 2004 - Award: \$50,000
- Feb 1996* Erasmus Fellowship of the European Community (EU) for Graduate Students
From February 12, 1996 to December 12, 1996

Research Projects

- 2006 – present **SHIPPER:** A community of UG and graduate students who will pursue advanced degrees in fields that combine expertise in high-performance computing and other scientific and engineering disciplines. <http://gcl.cis.udel.edu/projects/shipper>
- 2005 – present **DAPLDS:** A world-community experiment and effort to use distributed world-wide-web volunteer resources to assemble a supercomputer able to study putative drug compounds. <http://docking.cis.udel.edu>
- 2005 - present **Topaz:** An open-source GridFTP protocol extension to the Firefox browser that provides users with a familiar and user-friendly interface to access arbitrary GridFTP servers. <http://gcl.cis.udel.edu/projects/topaz>
- 2005 - present **RNAVLab:** A unified environment based on mathematical models and grid technology for computational RNA structure analysis, i.e., prediction, alignment, comparison, and classification. <http://navlab.utep.edu>
- 2004 – 2005 **Predictor@Home:** A world-community experiment and effort to use distributed world-wide-web volunteer resources to assemble a supercomputer able to predict protein structure from protein sequence. <http://predictor.scripps.edu>

Students and Mentoring Activities

Current Students:

Graduate Students

- Trilce Estrada (PhD student, Project: DAPLDS)
- Abel Licon (M.S. student, Project: DAPLDS)

Undergraduate Students

- Jason Parrott (Project: DAPLDS)
- Robert Keller (Project: DAPLDS)
- David Mireles (Project: RNAVLab, co-advised with Drs. Ming-Ying Leung and Thamar Solorio)

Graduated Students:

- David Flores (M.S., Computer Science, graduated Fall 2006, co-advised with Dr. Patricia J. Teller, title: "SimBA: A Discrete-event Simulator for Performance Prediction of Volunteer Computing Projects")
- Richard Zamudio (M.S., Computer Science, graduated Fall 2006, title: TOPAZ: A Firefox Protocol Extension for GridFTP " awarded with the Outstanding Thesis in the Department of Computer Science 2006-2007, now at Rockwell Collins, Iowa)

Graduate Committees:

- Jayaraman Suresh Babu (Principal supervisor: Patricia J. Teller), M.S., Computer Science, UTEP, 2006
- Maria Gabriela Aguilera (Principal supervisor: Patricia J. Teller), M.S., Computer Science, UTEP, 2005
- Yash Dayal (Principal supervisor: Gregory Lush), M.S., Electrical and Computer Eng., UTEP, 2005
- Javed Bilal Khan (Principal supervisor: John Chessa), M.S., Mechanical Engineering, UTEP, 2005

Other Mentored Students and Senior Personnel:

Undergraduate and Graduate Students:

- Daniel Catarino (BS UTEP, now at Exxon Mobile, GCL member: Spring 2006 - Fall 2006)
- Karina Escapita (BS UTEP, GCL member: Spring 2006 - Spring 2007)
- David Gomez-Leon (UG student UTEP, GCL member: Fall 2006 and Spring 2007)
- Abel Licon (BS UTEP, now graduate student at UDel, GCL member: Summer 2006 - Fall 2007)
- Guillermo Lopez (BS UTEP, not at Ximis - El Paso, Texas, GCL member: Fall 2006 and Spring 2007)
- Princess Trillo (UG student UTEP, GCL member: Spring 2007)
- Prayook Tungjatooronrusamee (MS UTEP - Leung and Tauffer, GCL member: Spring 2006 - Fall 2006)
- Vladimir Soto (UG student UTEP, GCL member: Spring 2007)

Research Staff:

- Roberto Araiza (PhD UTEP - Kreinovich, GCL member: Spring 2007 - Fall 2007)
- Andre Kerstens (MS UTDelf, now Systems Architect at SGI, GCL member: Spring 2006 - Spring 2007)

Undergraduate Mentoring:

Jan 2005 – May 2007 Mentor of approximately 40 undergraduate students at the Computer Science Department (UTEP). The mentoring includes individual meetings with each student on a semester basis to review their study progress and study plan.

Teaching Activities**Courses:**

- Spring 2008* CISC 849 - Analysis of Bio Simulations (Graduate course)
- Fall 2007* CISC 662 - Computer System: Architecture (Graduate course)
- Spring 2007* CS 5341 - Analysis and Modeling of Biological Structures (Graduate course – cross-listed with the Bioinformatics Program and the Chemistry Department)
- Spring 2007* CS 3320 – Computer Architecture II: Advanced Computer Design and Implementation (Undergraduate course)
- Fall 2006* CS 3335 – Systems Programming (Undergraduate course)
- Fall 2006* CS 3320 – Computer Architecture II: Advanced Computer Design and Implementation (Undergraduate course)
- Spring 2006* CS 3320 – Computer Architecture II: Advanced Computer Design and Implementation (Undergraduate course)
- Spring 2006* CS 5334 – Parallel and Concurrent Programming (Graduate course)
- Fall 2005* CS 3320 – Computer Architecture II: Advanced Computer Design and Implementation (Undergraduate course)
- Spring 2005* CS 5334 – Parallel and Concurrent Programming (Graduate course)

Professional Services and Activities

Conference Organization and Program Committee:

- Technical program committee of the Intl. Conference on Advanced Computing and Communications, December 2008, Chennai, India.
- Technical program committee of the ICCS 2008 conference, June 2008, Krakow, Poland.
- Technical program committee of the ACM Computing Frontiers 2008, May 2008, Ischia, Italy.
- Technical program committee of the Global and Peer-to-Peer Computing (GP2PC), May 2008, Lyon, France.
- Technical program committee of the 7th International Workshop on High Performance Computational Biology (HiCOMB 2008), May 2008, Miami, Florida, USA.
- Technical program committee of the 9th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC 2008), May 2008, Miami, Florida, USA.
- Technical program committee of the Second Workshop on Large-Scale, Volatile Desktop Grids (PCGrid 2008), May 2008, Miami, Florida, USA.
- Technical program committee of the 22th IEEE International Parallel and Distributed Processing Symposium (IPDPS 2008), May 2008, Miami, Florida, USA.
- Technical program committee of the Euromicro Conference on Parallel, Distributed and Network based Processing (PDP) February 2008, Toulouse, France.
- Technical posters Committee of the International Conference for High Performance Computing, Networking, Storage, and Analysis. November 2007, Reno, Nevada, USA.
- Technical program committee of the First Computational Structural Bioinformatics Workshop, November 2007, San Jose, California, USA.
- Poster Committee of the 2007 Richard Tapia Celebration of Diversity in Computing Conference, October 2007, Orlando, Florida, USA.
- Scholarship Committee of the Grace Hopper Celebration of Women in Computing 2007, October 2007, Orlando, Florida, USA.
- Technical program committee of the 5th IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA 2007), August-September, 2007, Niagara Falls, Ontario, Canada.
- Technical program committee of the International Conference on Computational Science 2007 (ICCS 2007), May 2007, Beijing, China.
- Technical program committee of the 6th International Workshop on Global and Peer-to-Peer Computing (GP2P 2007), May 2007, Rio de Janeiro, Brazil.
- Technical program committee for 26th IEEE International Performance Computing and Communications Conference (IPCCC 2007), April 2007 - New Orleans, Louisiana, USA.
- Technical program committee of the First Workshop on Large-Scale, Volatile Desktop Grids (PCGrid 2007), March 2007, Long Beach, California, USA.
- Technical program committee of the 4th IEEE International Symposium on Parallel and Distributed Processing and Applications (ISPA 2006), December 2006, Sorrento, Italy.
- Technical program committee of the Second IEEE International Conference on e-Science and Grid Technologies (eScience 2006), December 2006, Amsterdam, The Nederland.
- Technical program committee of the 5th IEEE International Workshop on High Performance Computational Biology (HiCOMB 2006), April 2006, Rhodes, Greece.
- Technical program committee of the 5th International Workshop on Global and Peer-to-Peer Computing (GP2P 2006), May 2006, Singapore.
- Technical program committee of the 20th IEEE International Parallel and Distributed Processing Symposium (IPDPS 2006), April 2006, Rhodes, Greece.
- Technical program committee of the 1st IEEE International Conference on e-Science and Grid Technologies (eScience 2005), December 2005, Melbourne, Australia.
- Technical program committee of the 2005 IEEE International Conference on Cluster Computing (Cluster 2005), September 2005, Boston, Massachusetts, USA.
- Technical program committee of the 2005 International Conference on High Performance Computing and Communications (HPCC 2005), September 2005, Sorrento (Naples), Italy.
- Technical program committee of the 5th International Workshop on Global and Peer-to-Peer Computing (GP2P 2005), May 2005, Cardiff, UK.
- Poster chair at the 9th Maria Goeppert-Mayer Symposium, San Diego Supercomputer Center, March 2004, La Jolla, California, USA.
- Technical program committee co-chair and organizer, First Advanced Topics Workshop on Desktop Grids:

Critical Systems and Applications Research (DGRID 2003). November 2003, Phoenix, Arizona, USA.

- Organization committee member, Joint Modular Languages Conference (JMLC 2000). September 2000, Zurich, Switzerland.

Conference Referee:

2008 PADS'08
 2007 PARA'07, SC'07
 2006 HPDC'06, Cluster'06, MCWC'06
 2005 SC'05, ICS'05
 2004 Cluster'04, HPDC'04
 2003 CCGrid'03, SC'03, Cluster'03

Journal Referee:

2007 IEEE Transactions on Information Technology in Biomedicine
 2006 Parallel Computing, Theory and Applications
 2005 IEEE Transactions on Parallel and Distributed Systems (IEEE-TPDS)
 2005 International Journal of Applied Intelligence

Services to Government Agencies:

Jul 2007 NSF, Curriculum, and Laboratory Improvement (CCLI) Program, Review Panel Member
 Feb 2006 - present Working group lead for the Multi-Scale Modeling Consortium (a collaboration between NIH, NSF, NASA, DoE). Goal of the working group is to discuss issues related to high performance computing, computational issues, and algorithms within the consortium. Webpage: <http://gcl.utep.edu/projects/msm>
 Aug 2006 Invited participant to the Workshop on Petascale Computing in the Biological Sciences, National Science Foundation (NSF)
 Mar 2006 NSF, CISE - Computer Systems Research (CSR) Program, Review Panel Member
 Mar 2005 NSF, CISE - Computer Systems Research (CSR) Program, Review Panel Member

Services to the University, College, and Department:

2007 - present Advisor for the student organization ACM Chapter for the Computer Science dept. at the University of Delaware
 2007 - present Member of the graduate recruiting committee at the University of Delaware
 2006 - 2007 Member of the Bioinformatics Research Committee and Bioinformatics Colloquium Committee (University level)
 2005 - 2007 Member of the High-End Computing Along the Rio Grande Consortium (University level). The committee organizes the annual participation of the four institutions in this consortium (UTEP, NMSU, UNM, and NMTech) to the exhibitor event at the International Conference for High Performance Computing and Communications (SC) conference.
 2005 - 2007 Member of the Computer System Curriculum Committee and the Facilities Committee (Department level)
 2006 Member of the NSF-CSEMS Scholarship Committee, 2006

Professional Affiliations:

- ACM, SIGMETRICS, ACM - Computing Reviews
- IEEE

Languages

- Native language: Italian
- Fluent in English and German

Inverting Middleware: Performance Analysis of Layered Application Codes in High Performance Distributed Computing

**Abstract of the Doctoral Thesis of Michela Taufer
Swiss Federal Institute of Technology Zurich (ETH), Switzerland**

Many important application codes were developed for vector supercomputers and SMP machines. In the last decade, the computing research has moved away from such expensive platforms to cheaper distributed systems such as clusters of PCs. Further on, the migration of these application codes to widely distributed systems, on so called desktop computational grids, looks tempting. Re-engineering applications for such distributed systems while at the same time maintaining good performance remains a challenging task, since we are still lacking tools and instrumentation for performance analysis that work well together with standard middleware. While middleware packages help the application writer to reduce the programming effort, they still cause some loss of control over performance issues that results in suboptimal usage of the machine resources.

To address this problem, we propose a novel method for performance analysis including a framework called inverted middleware. The inverted middleware assists the process of performance engineering by mapping low level performance information, monitored at the operating system layer, back to a higher level, i.e., the application layer. For a distributed system, our inverted middleware framework comprises software instrumentation at the OS level, tools for gathering relevant performance data and an analytical model for performance prediction on distributed systems. The inverted middleware is used side by side with the middleware packages.

We demonstrate the viability of our approach with the performance analysis of the scientific code DYANA for molecular dynamics and a standard OLAP (OnLine Analytical Processing) application, the TPC-D benchmark. With the inverted middleware, we provide a detailed performance characterization of different workloads according to their resource usage, quantify the scalability for new alternative platforms and investigate the impact of the network on the overall application performance. This information helps an expert to effectively re-engineer and successfully migrate application software to new platforms.

References

Patricia (Pat) J. Teller

Professor
Computer Science Department
College of Engineering
University of Texas at El Paso
500 W. University Ave
El Paso, Texas 79968

Phone: (915) 747-5939
E-mail: pteller@utep.edu

Ming-Ying Leung

Professor
Director of Bioinformatics Program
Department of Mathematical Sciences
University of Texas at El Paso
500 W. University Avenue
El Paso, Texas 79968

Phone: (915) 747-6836
E-mail: mleung@utep.edu

Karan Bhatia

Group Leader for the Grid Development group
San Diego Supercomputer Center
University of California, San Diego
9500 Gilman Drive
La Jolla, California 92093

Phone: (858) 534-5019
E-mail: karan@sdsc.edu

Kim Baldrige

Professor
Organic chemistry Institute (OCI)
University of Zürich
Winterthurestrasse 190
8050 Zurich, Switzerland

Phone: +1 41 1 63 54201
E-mail: kimb@oci.unizh.ch

Charles L. Brooks III

Professor
Department of Molecular Biology, TPC6
The Scripps Research Institute
10550 North Torrey Pines Road
La Jolla, California 92037

Phone: (858) 784-8035
E-mail: brooks@scripps.edu

David P. Anderson

Research Scientist
U.C. Berkeley Space Sciences Laboratory
University of California at Berkeley
7 Gauss Way
Berkeley, California 94720

Phone: (510) 642-4921
E-mail: davea@ssl.berkeley.edu

Andrew A. Chien

Director, Intel Research
INTEL CORPORATION

Phone: (858) 822-2458
E-mail: achien@ucsd.edu